

Entanglement manipulation by a magnetic pulse in $Gd_3N@C_{80}$ endohedral metallofullerenes on a $Cu(001)$ surface

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In this paper we present result of theoretical calculation of entanglement within a spin structure of $Gd_3N@C_{80}$ under the influence of rectangular impulses. Research is conducted using general spin Hamiltonian within SSNQ (spin system of N-qubits). Calculation of entanglement with variable impulse is performed using the time-dependent Landau-Lifshitz-Gilbert equation with spin-spin correlation function. We show that long rectangular impulse ($t=850ps$) can be used for maintaining of entanglement value. This allows us to offer a new algorithm which can be used to reduce the challenge of decoherence to logical scheme optimization.

PACS numbers:

I. INTRODUCTION

Quantum entanglement plays a central role in quantum information and quantum computation.^{1,2} Though the theoretical investigations of the magnetism and electronic structure of lanthanides have been performed decades ago at the same time fundamental results of the time dependent spin structure appear under a new light how a molecular spintronics.³ Quantum entanglement (QE) also exists on the nanoscale in solid state and molecular systems.⁴ Condensed matter systems are especially interesting subjects for studying entanglement, f.e. entanglement of spins, for several reasons. First and foremost, condensed matter is the basis of a sizeable portion of today's research and development in spintronics and information industries. Understanding QE in solids and nanostructures could open a complete new perspective on those research directions. Moreover, the source of QE of spin states is the exchange interaction, which is known to be strong in condensed matter systems.⁵ In the case of solids and molecules, however, detecting QE can be tricky.

Key challenges in building a quantum computer from spin qubits in physical systems are preparation of arbitrary spin states, implementation of the arbitrary qubit evolution, reading out the qubit states, overcoming of the decoherence and doing all this on a large scale; that is, with a large number of qubits or a spin system of N-qubits (SSNQ) with the definite spin structure.⁵ For the purposes of implementing quantum computation, the physical system can be treated as a SSNQ in which the couplings between the qubits can be controlled externally. The concept of a SSNQ can be related to the problem of the quantum spin structure, where the nontrivial applications may exist for computers with a limited number N of a qubits. The precise relationship between the type

of the entanglement and the distribution of the coupling strengths in the SSNQ can be strongly dependent on external parameters, such as applied magnetic pulse fields. In this context, systematic studies of the relationship between the quantity and nature of the entanglement and the spin structure of the SSNQ via magnetic pulse has been pursued in order to identify the optimal spin structures to create specific types of the entanglements. Here we use the spin correlating states⁶ to study entanglement in metallic clusters of Gd trimers in $Gd_3N@C_{80}$ endohedral metallofullerene on a $Cu(001)$ surface⁷.

The relevance of the $Gd_3N@C_{80}$ molecular magnet under a magnetic pulses to be considered for qubits perspectives will be discussed in this paper. For this purpose the time-dependent spin dynamics is involved within a micro-magnetic model based on the general spin Hamiltonian (GSH) formalism, where the spin is considered as a spatial and time-dependent continuous function. In this case the dynamics of spins obeys the Landau-Lifshitz-Gilbert (LLG) equation⁸, involving the various energy contributions from the exchange, magnetostatic and Zeeman interactions, and magnetic anisotropy of the spin system. It is known, that correlations are of a great importance in the study of spin systems. They are directly related to the entanglement between different atomic spins, which can be employed in the field of quantum information processing. Therefore entanglement arising in the correlated quantum spin systems has become one of the most widely investigated phenomenon in quantum physics during last years. Now it is well known how to create entanglement in quantum spin systems, but how it propagates inside a system is still an important fundamental question in quantum information theory. Therefore the theoretical descriptions of the time-dependent properties of the correlated quantum spin systems is very important nowadays. Recently it was claimed, that the controlled and manip-

ulated entanglement in the quantum spin systems could be realized precisely and effectively by means of the required dynamical operations in presence of the magnetic pulse.⁹ Moreover, it was shown also that the solid state spin-based system with a definite spin structure can be considered as a spin system of N-qubits, which demonstrates the prolonged time of the decoherence demanded for quantum information processing. For implementation of quantum computation one can treat a quantum spin system as a SSNQ, where the couplings between the spin qubits can be controlled externally, for instance by the applied magnetic pulse. Therefore the systematic studies of inherent relationship between the strength of the entanglement and the peculiarities of spin structure of a SSNQ are carried out in order to find the optimal time-dependent spin structures with specific types of the controlled and engineered entanglements.

II. THE THEORETICAL APPROACH

A. The spin-dynamics simulations

The dynamic behavior of a spin is determined by the equation of motion, which can be derived from the quantum theory with the spin Hamiltonian \hat{H}_{spin} that calculated the spin structure of a magnetic cluster with Hamiltonian

$$\hat{H}_{spin} = \hat{H}_{ex} + \hat{H}_{an} + \hat{H}_{ZEE} + \hat{H}_a(t). \quad (1)$$

The first term \hat{H}_{ex} is the Heisenberg Hamiltonian, which represents the isotropic exchange interaction, H_{an} is the exchange Hamiltonian the term due to the axial single-ion anisotropy, and H_{ZEE} is the interaction between the spin system and the external magnetic field. This Hamiltonian, which describes the interaction of the spin $\hat{\mathbf{S}}$ with the external magnetic field, given by its flux \mathbf{H}_{eff} , can be expressed as:

$$\hat{H}_{spin} = -\mathbf{H}_{eff}\hat{\mathbf{S}} \quad (2)$$

where the effective magnetic field \mathbf{H}_{eff} is an external magnetic field \mathbf{H}_z , the anisotropy fields \mathbf{H}_{an} , the exchange interaction \mathbf{H}_{ex} and external magnetic pulse field $\mathbf{H}_{pulse}(t)$. Here we use the approximation for $\mathbf{H}_{eff} \Rightarrow \mathbf{H}_{eff}^{mean}$ with replacement $\hat{\mathbf{S}} \Rightarrow \mathbf{M}_s = \gamma\langle\hat{\mathbf{S}}\rangle$. Use¹⁰ we obtain that

$$\frac{\partial\langle\hat{\mathbf{S}}\rangle}{\partial t} = \frac{1}{1+\lambda^2}\langle\hat{\mathbf{S}}\rangle \times \mathbf{H}_{eff}^{mean} - \frac{\lambda}{1+\lambda^2}\langle\hat{\mathbf{S}}\rangle \times (\langle\hat{\mathbf{S}}\rangle \times \mathbf{H}_{eff}^{mean}) \quad (3)$$

The effective magnetic field \mathbf{H}_{eff}^{mean} is given by the free magnetic energy variational with magnetization:

$$\mathbf{H}_{eff}^{mean}(\mathbf{M}_s, t) = -\frac{\delta F}{\delta \mathbf{M}_s},$$

where F is the free energy of the magnetic nanosystem. The effective field \mathbf{H}_{eff}^{mean} can be derived from the free

energy functional

$$\mathbf{H}_{eff}^{mean} = -\frac{\delta(F(\mathbf{M}_s, H_z) + F(t))}{\delta \mathbf{M}_s} = -\frac{\partial F(\mathbf{M}_s, H_z)}{\partial \mathbf{M}_s} + H_{pulse}^x(t), \quad (4)$$

We have derived a general form of the time-dependent spin equation for a system of the spins precessing in an effective magnetic field with specifying the interactions in the magnetic cluster on a surface.

A spin structure is defined only proceeding from the spin model of a cluster. Here we use to calculate a spin structure by the ITO method within the generalized spin Hamiltonian \hat{H}_{spin} .

Since in further researches the anisotropic part of a cluster will be only scalar, the magnetic properties of the anisotropic system do not depend on the direction of the magnetic field. Thus we can consider the external magnetic field H_z directed along arbitrary axis z of the cluster coordinate frame that is chosen as a spin quantization axis. In this case the energies of the system will be $\epsilon_\mu(\mathbf{M}_s) + g_e M_s H_z$, where $\epsilon_\mu(\mathbf{M}_s)$ are the eigenvalues of the spin-Hamiltonian containing the magnetic exchange and the double exchange contributions (index μ runs over the energy levels with given total spin protection \mathbf{M}_s).

We use them further to define the spin-spin correlation functions \mathcal{C}_{ij} for the entangled ground state $|SM_0^{(ij)}\rangle = \alpha_i |SM\rangle_i + \beta_j |SM\rangle_j$ of the system⁷:

$$\mathcal{C}_{ij}^{\alpha\beta}(t) = \langle SM_0^{(ij)} | \hat{S}_i^\alpha(t) \hat{S}_j^\beta(t) | SM_0^{(ij)} \rangle = \langle S_i^\alpha(t) \rangle \langle S_j^\beta(t) \rangle, \quad (5)$$

where $\alpha, \beta \in x, y, z$.

The ground state is in the subspace \mathcal{A} for which $M^{(\mu)} = 0$ for all μ .

The entanglement entropy between a subspace \mathcal{A} and the rest of the system \mathcal{R} is given by:

$$S_{\mathcal{A}} = -\text{Tr}(\rho_{\mathcal{A}} \log_2 \rho_{\mathcal{A}}), \quad (6)$$

where $\rho_{\mathcal{A}}$ is the reduced density matrix of the subspace \mathcal{A} obtained by tracing out over all those parts of the Hilbert space not associated with \mathcal{A} . We consider the subspace $\mathcal{A}_{ij} \equiv \{i, j\}$ consisting of all spin pairs (not only neighboring) i and j of the ground states $|S^{(\mu)} M^{(\mu)} = 0\rangle$ ¹². For the rest of the system \mathcal{R} is given by $\mathcal{R}_{kl} \equiv \{k, l\}$. The matrix elements of the reduced density matrix, needed to calculate the entanglement, can be written in terms of the spin-spin correlation functions $\mathcal{C}_{ij}^{\alpha\beta}(t)$ (see eq. (5)):

$$\rho_{\mathcal{A}}^{(ij)}(t) = \sum_{\alpha, \beta \in x, y, z} \langle SM_0^{(ij)} | \hat{S}_i^\alpha(t) \hat{S}_j^\beta(t) | SM_0^{(ij)} \rangle \rho_{\mu\nu}^{(ij)}, \quad (7)$$

where

$$\rho_{\mu\nu}^{(ij)} = |SM_0^{(ij)}\rangle_\mu \otimes |SM_0^{(ij)}\rangle_\nu.$$

Suppose $\{|\mathcal{A}_{ij}\rangle\}$ and $\{|\mathcal{R}_{kl}\rangle\}$ are the orthonormal basis states of the many-body Hilbert space of the subsystems \mathcal{A} and \mathcal{R} . A general quantum spin state of the composite system can be described by wave function[?]:

$$|\Psi\rangle = \sum_{ij,kl} C_{ij,kl} |\mathcal{A}_{ij}\rangle |\mathcal{R}_{kl}\rangle. \quad (8)$$

Here, a rectangular matrix \mathbf{C} can be presented always in the form $\mathbf{U}\mathbf{D}\mathbf{V}^\dagger$, where \mathbf{U} is unitary, \mathbf{D} is diagonal and the rows of \mathbf{V} are orthonormal. It is known already as the singular-value decomposition (SVD). Using this decomposition in eq. (8) and forming a new basis by combining the $|\mathcal{A}_{ij}\rangle$ with \mathbf{U} and the $|\mathcal{R}_{kl}\rangle$ with \mathbf{V}^\dagger , one can obtain the Schmidt decomposition[?]:

$$|\Psi\rangle = \sum_{k=1}^{Rank} \sigma_k |\Phi_k^{\mathcal{A}}\rangle |\Phi_k^{\mathcal{R}}\rangle, \quad (9)$$

which represents the total wave function $|\Psi\rangle$ of the system as a single sum of products of the orthonormal functions. Here the *Rank* number of the terms is limited by the smallest one of the two Hilbert spaces and the weight factors σ_k are the matrix elements of the diagonal matrix \mathbf{D} . If $|\Psi\rangle$ is normalized, their absolute magni-

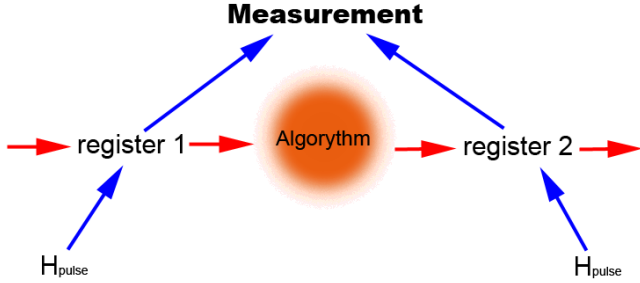


FIG. 1: Principle of "reload"

tudes squared sum to one. The entanglement properties of a system are performed with the set of σ_k :

$$S_{\mathcal{A}}(t) = - \sum_{k=1}^{Rank} \tau_k(t) \log_2 \tau_k(t), \quad (10)$$

where

$$\tau_k(t) = \langle S_i^\alpha \rangle(t) \langle S_j^\beta \rangle(t) \sigma_k^2. \quad (11)$$

III. RESULTS AND DISCUSSIONS

Quantum entanglement is primary criteria of quantum computer efficiency. Due to that fact retention of entanglement for a long time is main challenge facing researchers. This problem calls decoherence. A great number of increase the coherence time methods for circumvent this phenomenon are invented. But all of these algorithms cannot completely eliminate decoherence.

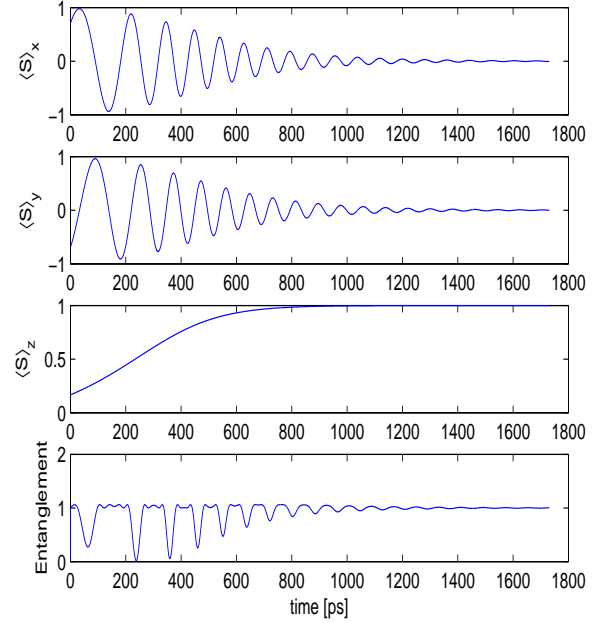


FIG. 2: (Color online) The evolution of the time-dependent quantum mechanical expectations $\langle S^{x,y,z} \rangle(t)$ of the $Gd_3N@C_{80}$ molecule under magnetic pulses $H_{pulse}=0T$.

We offer a new method in which entanglement maintained by two long rectangular pulses. It allows us to hold maximal measure of quantum entanglement until pulse affect on system. Within a framework of this method we create an algorithm of quantum computer efficiency maintenance that operate under a principle of "reload" (Fig. 1). At first step by the long rectangular pulse we create entanglement and maintain maximal value of it. During the pulse wave functions of system is measured. At the second step we impact on system by operators of scheme. At the third step of algorithm we do measurement of system wave functions and create a maximal entanglement by the second long rectangular pulse. Due to the fact that this algorithm can be used as a cycle entanglement is maintained on maximal value, it changes only in second step. The priority in this method is not coherence during the quantum computer working time but coherence within work of scheme. This allows us to reduce the challenge of decoherence to scheme optimization which is a solvable problem. We studied endohedral

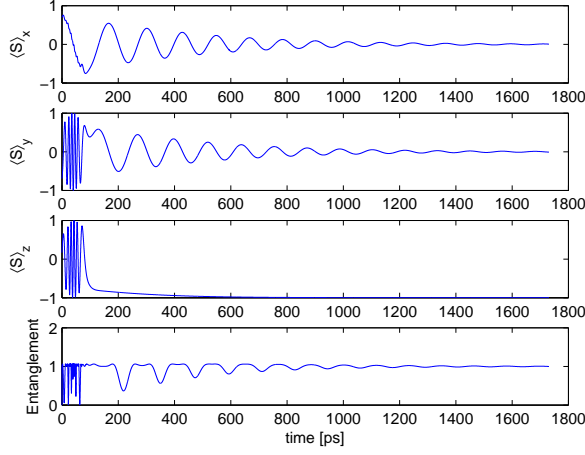


FIG. 3: (Color online) The evolution of the time-dependent quantum mechanical expectations $\langle S^{x,y,z} \rangle(t)$ of the $Gd_3N@C_{80}$ molecule under magnetic Gauss pulses $H_{pulse}=5.3T$.

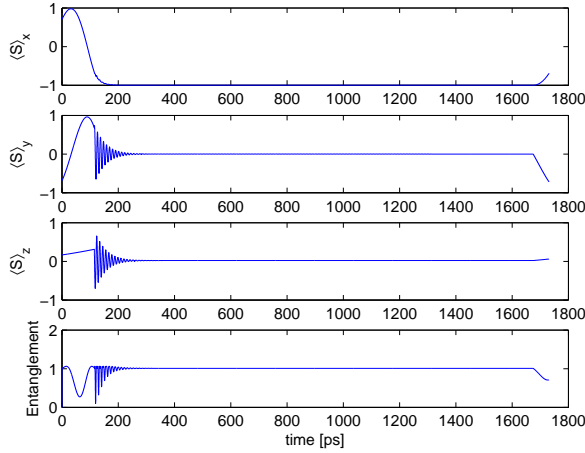


FIG. 4: (Color online) The evolution of the time-dependent quantum mechanical expectations $\langle S^{x,y,z} \rangle(t)$ of the $Gd_3N@C_{80}$ molecule under magnetic rectangular pulses $H_{pulse}=5.3T$.

fullerene $Gd_3N@C_{80}$ due to the antiferromagnetic coupling between the encapsulated magnetic moments and the electrons situated on the carbon cage. This property makes this compound promising candidate for molecular spintronics.

Entanglement of system without impulse impact (Fig. 2) is unstable. That's why probability of decoherence during computing is high. Short rectangular impulse ($H_{pulse}=5.3T$, $t=200ps$) is the cause of spin-switching (Fig. 3). Due to that effect (which is reviewed by Far-

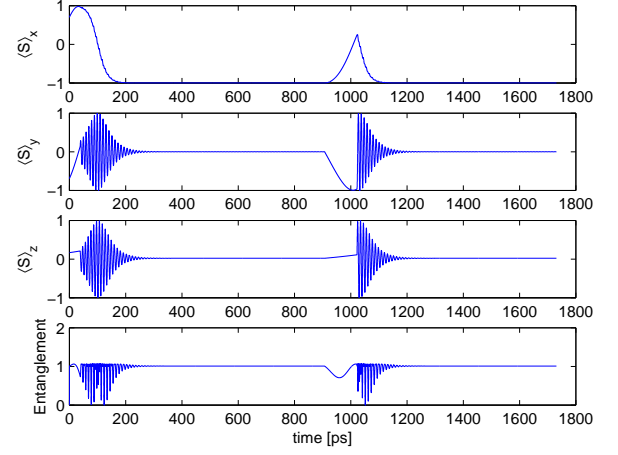


FIG. 5: (Color online) The evolution of the time-dependent quantum mechanical expectations $\langle S^{x,y,z} \rangle(t)$ of the $Gd_3N@C_{80}$ molecule under two magnetic rectangular pulses $H_{pulse}=5.3T$.

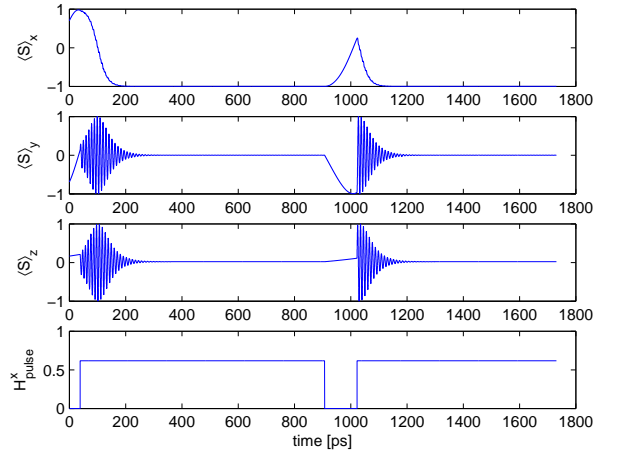


FIG. 6: (Color online) The evolution of the time-dependent quantum mechanical expectations $\langle S^{x,y,z} \rangle(t)$ of the $Gd_3N@C_{80}$ molecule under two magnetic rectangular pulses $H_{pulse}=5.3T$.

berovich O.V.) it is possible to create quantum gates and logical schemes. Impact of long rectangular impulse ($H_{pulse}=5.3T$, $t=1400ps$) on system leads to very interesting results. During this impulse entanglement was maintained on maximal value. This behavior of quantum system shows us that long rectangular impulse can increase a coherence time (Fig. 4). Results of two long rectangular impulses ($H_{pulse}=5.3T$) impact shown on Fig. 5 (influence of impulses at system) and 6 (long rectangular impulses duration). Value of entanglement is maintained on maximum level during first and second impulses ($t=850ps$) and decrease only between them. We offer to impact to system by logical scheme in this mo-

ment.

IV. CONCLUSION

In present paper we consider a results of entanglement of endohedral fullerene $Gd_3N@C_{80}$ theoretical analysis. Calculation performed with exchange integrals from paper⁷. We show that long rectangular impulse ($H_{pulse}=5.3T$) with duration 850ps can be used for maintaining of entanglement on maximal value. Due to this

fact it has become possible to reduce problem of decoherence in quantum computers to challenge of logical scheme optimization by using a two long rectangular impulses with $H_{pulse}=5.3T$ and $t=850ps$ each.

Acknowledgments

The part of this research has been supported by Russian Ministry of Science, Grant RFMEFI 58714X0002.

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